

Claims

- [c1] 1. A user accessible chemical design and query tool, comprising:
a user interface;
a database storing:
a graphical representation of at least one chemical design structure;
wherein, upon accessing said chemical design and query tool by a user, said user interface guides said user in selecting a chemical design structure and submitting said chemical design structure to a provider system.
- [c2] 2. The user accessible chemical design and query tool of claim 1, further comprising:
a graphical representation of at least one chemical backbone structure; and
a graphical representation of at least one chemical substituent selectable for said at least one chemical backbone structure, said chemical substituent operable for specifying a custom chemical design structure;
wherein, upon accessing said chemical design and query tool by a user, said user interface guides said user in selecting a chemical backbone structure, attaching said graphical representation of said at least one chemical substituent to a selected chemical backbone structure, and submitting a resulting custom chemical design structure to a provider system.
- [c3] 3. The user accessible chemical design and query tool of claim 2, further comprising:
a text window operable for providing comments and further specifying said custom chemical design structure.
- [c4] 4. The chemical design and query tool of claim 2, further comprising:
at least one R group included in said graphical representation of at least one chemical backbone structure, wherein said R group specifies a permissible location for attaching said at least one chemical substituent.
- [c5] 5. The chemical design and query tool of claim 2, further comprising an interactive host.
- [c6] 6. The chemical design and query tool of claim 2, wherein said at least

one chemical substituent comprises at least one chemistry.

- [c7] 7. The chemical design and query tool of claim 2, wherein said chemical backbone structure is classified by at least one of:
organic; and
inorganic.
- [c8] 8. The chemical design and query tool of claim 5, wherein said interactive host guides said user in operating said tool.
- [c9] 9. The chemical design and query tool of claim 8, wherein said interactive host is animated, including a capability to take on a plurality of positions and poses.
- [c10] 10. The chemical design and query tool of claim 8, wherein said interactive host communicates with said user via at least one of:
speech;
sound;
text bubbles;
animated movements; and
changes in color and facial expression.
- [c11] 11. The chemical design and query tool of claim 5, wherein a user selects said interactive host from a plurality of interactive host choices.
- [c12] 12. The chemical design and query tool of claim 4, wherein a chemical substituent is assigned to an R location by said tool as a default in the event that no chemical substituents were attached by said user.
- [c13] 13. The chemical design and query tool of claim 2, wherein said custom chemical design structure is created and edited utilizing interface techniques including at least one of:
a linear click-thru application operable for allowing a user to add or modify a structure one step at a time using HTML select boxes;
dynamic HTML technology operable for allowing a user to select an animated molecule, click on a desired structural change, resulting in a distinct structure;
a multi-dimensional graphics component operable for allowing multi-

dimensioned viewing of a structure; and
a structure/function feature operable for:
viewing properties associated with a backbone structure;
viewing properties associated with a chemical substituent; and
previewing additional properties that would be added to a backbone structure,
if a specified substituent was attached to said backbone structure.

[c14] 14. The chemical design and query tool of claim 2, wherein said chemical backbone structure includes a silicone backbone palette comprising:
small molecule silanes;
cyclic silicones; and
polymeric materials including linear silicones and branched silicones.

[c15] 15. A system for designing and locating chemical structures, comprising:
a host system comprising:
a server;
a data storage device housing a customer database, a chemical database, and a workflow database, said data storage device accessible to said server;
a chemical design and query tool executable by said server, said chemical design and query tool including a user interface; and
a workflow component; and
a link to at least one user system;
wherein said host system tracks queries resulting from custom chemical design structures created and submitted by user systems via said chemical design and query tool, and searches said chemical database for a compatible chemical structure and, depending upon search results, provides an autoresponse message to said user systems and performs related tracking activities via said workflow component.

[c16] 16. The system of claim 15, further comprising a link to a vendor network system, said link operable for facilitating communication between said user system and at least one entity of said vendor network system, wherein said host system provides a link to a URL for said vendor network system upon finding a potential match to said queries.

[c17]

17. The system of claim 15, wherein said workflow component includes a summary screen operable for facilitating tracking activities of queries, said summary screen comprising at least one of:

- a case number assigned to each query;
- an assignment of said query to a designated entity or individual;
- customer registration data;
- customer contact data;
- query data including:
- application data;
- backbone type;
- R group data; and
- user comments; and

workflow and tracking information operable for assisting technical specialists, administrative personnel and gatekeepers of said host system in processing said query.

[c18]

18. A method for designing and locating chemicals via a chemical design and query tool, comprising:

- receiving a welcome screen upon accessing said chemical design and query tool;
- selecting a type of chemical backbone operable for serving as a basis for a chemical query;
- selecting and attaching at least one chemical substituent to said chemical backbone resulting in a custom chemical design; and
- submitting a resulting custom chemical design query to a host system.

[c19]

19. The method of claim 18, further comprising an interactive host, said interactive host prompting a user through designing a custom chemical design structure.

[c20]

20. A method for designing and locating chemicals via a chemical design and query tool, comprising:

- receiving a welcome screen upon accessing said chemical design and query tool;

utilizing a drag and drop software routine:
selecting a type of chemical backbone operable for serving as a basis for a chemical query; and
attaching at least one chemical substituent to said chemical backbone resulting in a custom chemical design; and
submitting a resulting custom chemical design query to a host system.

[c21] 21. A method for designing and locating chemicals via a chemical design and query tool, comprising:
receiving a welcome screen upon accessing said chemical design and query tool;
utilizing a drop down software routine:
selecting a type of chemical backbone operable for serving as a basis for a chemical query; and
attaching at least one chemical substituent to said chemical backbone resulting in a custom chemical design; and
submitting a resulting custom chemical design query to a host system.

[c22] 22. A method for tracking custom chemical design queries, comprising:
receiving a custom chemical design query from a user system;
routing said query to a gatekeeper at a computer processing device or central storage location, said gatekeeper representing an initial point of contact for said query;
comparing data in said query with existing chemical structures;
if a match is found, transmitting a first autoresponse message to said user system;
if no match is found, comparing said query with structures available in a vendor network system;
if a match is found in said vendor network system, transmitting a second autoresponse message to said user system;
if no match is found in said vendor network system, determining whether tolling is an option;
if tolling is an option, transmitting a third autoresponse message to said user system; otherwise, transmitting a fourth autoresponse message to said user

system.

[c23] 23. A storage medium encoded with machine readable computer program code for designing and locating chemicals via a chemical design and query tool, said storage medium including instructions for causing said tool to implement a method comprising:

- receiving a welcome screen including an interactive host upon accessing said chemical design and query tool;
- selecting a type of chemical backbone operable for serving as a basis for a chemical query;
- selecting and attaching at least one chemical substituent to said chemical backbone; and
- submitting a resulting custom chemical design query to a host system.

[c24] 24. The storage medium of claim 23, further comprising instructions for causing said computer to implement:

- prompting a user through designing a custom chemical design structure utilizing an interactive host.

[c25] 25. A storage medium encoded with machine-readable computer program code for tracking custom chemical design queries, said storage medium including instructions for causing said computer to implement a method comprising:

- receiving a custom chemical design query from a user system;
- routing said query to a gatekeeper at a computer processing device or central storage location, said gatekeeper representing an initial point of contact for said query;
- comparing data in said query with existing chemical structures;
- if a match is found, transmitting a first autoresponse message to said user system;
- if no match is found, comparing said query with structures available in a vendor network system;
- if a match is found in said vendor network system, transmitting a second autoresponse message to said user system;
- if no match is found in said vendor network system, determining whether tolling

